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Study of superconductivity and antiferromagnetism gaps in cuprates

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Abstract : The high T_c superconductor exhibits very interesting co-existence of anti-ferromagnetism (AFM) and superconductivity (SC) in its doped state. The electron doped Nd- and hole doped La- cuprate systems show varieties of exotic properties. In this communication we report a theoretical model to explain the origin of co-existence of SC and AFM gaps in the doped systems through self-consistent numerical analysis of both the gaps and their corresponding density of states (DOS). The impurity *f*-level of the Nd and La lie on the Fermi level ($\epsilon_F = 0$) and there exists a weak hybridization between the f-level and the 3*d* electron of copper. The copper sites are represented by two sub-lattice sites 1 and 2 to simulate insulating sub-lattice staggered magnetic field. The DOS shows the interplay of SC, AFM and hybridization gaps for different parameters at various temperatures. Further the various amplitudes are calculated to investigate the temperature gap anomalies. The results are discussed.

Keywords : Superconductivity, antiferromagnetic order.

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1. Introduction

Out of several high T_c super-conductors. ($R_{2-x}MxCuO_4$) (R = Nd, Pr,..; M = Sr, Ce, ...) compounds have received a considerable amount of attention, because they become electron carrier super-conductors [1]. When Nd_2CuO_4 is doped with Ce impurity, it changes its insulating phase to the semi-conducting phase with Ce con-centration x~0.10. The extra electron of Ce enters into Cu-O plane and gives rise to SC at x = 0.15. This super-conducting phase co-exists with anti-ferromagnetic ordering. This phase is very interesting to explore the pairing mechanism of SC. The Ce impurity decreases the separation between planar copper and apexial oxygen atoms and increases the separation between planar copper and oxygen atoms. As a result, the impurity introduces electron-phonon interaction and lattice distortion. It will be interesting to study the co-existence of SC and magnetism in the presence of lattice distortion [2]. At a concentration of 0.20, the metallic phase exists where a linear specific heat term with coefficient γ = 4000 mJ/K^2/mol of Nd is observed [3]. This is a new prototype heavy fermion material resulting probably due to coupling between Nd moments and copper spins. In the present communication, we attempt to study the interplay between

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SC and AFM impurity f-electrons and also through different pairing amplitudes.

2. Theoretical model

In the hole doped La-system and electron doped Nd-system, the anti-ferromagnetic exchange usually leads to the Néel group state which is characterized by a long-range anti-ferromagnetic order in the spin alignment on Cu lattice sites. Hence the copper lattice is divided into two sub-lattices 1 and 2. For this system a model is proposed by fulde [3,4] to describe the normal phase and Panda *et al* [1] have extended this model for the doped superconducting phase. The Hamiltonian used in this model is given by

$$H_o = H_d + H_s + H_\upsilon + H_f\ , \tag{1}$$

where H_d describes the Hamiltonian involving hopping of copper d-electron between adjacent sites is given by

$$H_d = \sum \epsilon_0(k)\left(a^\dagger_{k\sigma} b_{k\sigma} + hc\right). \tag{2}$$

Here, $a^\dagger_{k\sigma}, b_{k\sigma}$ and $f^\dagger_{k\sigma}$ are the creation operatures of electrons at sites 1 and 2 of copper and f-level, respectively. The hopping takes place between the neighboring sites of copper with dispersion $\epsilon_0(k) = 2t_0(\cos k_x + \cos k_y)$. We introduce a staggered magnetic field of strength 'h' which simulates strong AFM correlation of copper d-electron. This can be written as

$$H_s = (h/2)\sum_{k\sigma} \sigma\left(a^\dagger_{k\sigma} a_{k\sigma} - b^\dagger_{k\sigma} b_{k\sigma}\right). \tag{3}$$

The staggered magnetic field h is given by

$$h = -\frac{1}{2} g\mu_B \sum_{k\sigma}\left[\left\langle a^\dagger_{k\sigma} a_{k\sigma}\right\rangle - \left\langle b^\dagger_{k\sigma} b_{k\sigma}\right\rangle\right], \tag{4}$$

where g and μ_B are Lande g-factor and Bhor magnetron. The Hamiltonian describing the hybridization between the f-level and copper d-band is given by

$$H_\upsilon = V\sum_{k,\sigma}\left(a^\dagger_{k,\sigma} f_{1,k,\sigma} + b^\dagger_{k,\sigma} f_{2,k,\sigma} + hc\right). \tag{5}$$

The intra f-electron Hamiltonian is given by

$$H_f = \epsilon_f \sum_{k,\sigma}\left(f^\dagger_{1,k,\sigma} f_{1,k,\sigma} + f^\dagger_{2,k,\sigma} f_{2,k,\sigma}\right), \tag{6}$$

where ϵ_f is the dispersionless renormalized f-level energy of the rare-earth ion and $f^\dagger_{i,k,\sigma}(f_{i,k,\sigma})$ is the creation (annihilation) operator of the localized electron in the sublattice i = I, 2. Finally, the BCS type mean-field Hamiltonian describing superconductivity through some mediation other than phonon exchange at two different sites of copper (assuming only intra sub-lattice pairing) is given by

$$H_I = -\Delta\sum_k\left[\left(a^\dagger_{k,\uparrow} a^\dagger_{-k,\downarrow} + b^\dagger_{k,\uparrow} b^\dagger_{-k,\downarrow} + hc\right)\right]. \tag{7}$$

Though it is well known that the high T_c superconductor show *d*-wave pairing, we have considered here *s*-wave pairing in order to study the interplay between superconductivity and anti-ferromagnetism for simplicity. It is to be noted that the total Hamiltonian of the system is a mean field one which can be solved exactly.

3. Expression for SC gap and staggered field

One electron Green's functions are calculated using the Hamiltonian given in eq. (1) for the superconducting state of the cuprate system by using Zubarev's technique [5]. A set of six coupled Green's functions are solved to find out the long range order parameters. The superconducting gap $\Delta(T)$ and the staggered magnetic field are calculated from the Green's functions and are given below.

$$\Delta(T) = -\sum_{k} \bar{V}_k \left[\left\langle a^{\dagger}_{k,\uparrow} a^{\dagger}_{-k,\downarrow}\right\rangle + \left\langle b^{\dagger}_{k,\uparrow} b^{\dagger}_{-k,\downarrow}\right\rangle\right], \tag{8}$$

$$\Delta(T) = V_0 N(0) \int_{-\omega_D}^{\omega_D} d\epsilon_0(k) \left[F_1(k,T) + F_2(k,T)\right], \tag{9}$$

where

$$F_1(k,T) = \frac{\Delta - h/2}{2\sqrt{E_{1k}^4 - 4V^4}} \left[\omega_1 \tanh\frac{\beta\omega_1}{2} - \omega_2 \tanh\frac{\beta\omega_2}{2}\right.$$

$$F_2(k,T) = \frac{\Delta + h/2}{2\sqrt{E_{2k}^4 - 4V^4}} \left[\omega_3 \tanh\frac{\beta\omega_3}{2} - \omega_4 \tanh\frac{\beta\omega_4}{2}\right. \tag{10}$$

The quasi particle energy bands $\pm\omega_i\,(i = 1-4)$, which are given by

$$\pm\omega_{1,2} = \left[\frac{E_{1k}^2 \pm \sqrt{E_{1k}^4 - 4V^4}}{\quad}\right]^{1/2}$$

$$\pm\omega_{3,4} = \left[\frac{E_{2k}^2 \pm \sqrt{E_{2k}^4 - 4V^4}}{\quad}\right]^{1/2} \tag{11}$$

The final expression for the staggered magnetic field is

$$h = -g_1 \int_{W/2}^{-W/2} d\epsilon_0(k) \left[F_1(k,T) - F_2(k,T)\right]. \tag{12}$$

4. Calculation for pairing amplitudes and density of states

In order to study interplay of the superconducting (SC) and antiferromagnetism (AFM), the gap parameters Δ and h are solved self-consistently under the half-filled band situations. Further, it is assumed that the impurity *f*-level lies on the Fermi-level (*i.e.* $\epsilon_F = 0$). This interplay of AFM and SC shows anomalies as reported in the calculations [1] at low temperatures. In order to explain the low temperature anomalies, we have calculated the relevant mixed pairing amplitudes and hybridization parameters.

It is observed that the mixed superconducting pairing amplitude like $\left\langle a^{\dagger}_{k,\uparrow} b^{\dagger}_{-k,\downarrow}\right\rangle$ comprising of inter-site operators of copper sublattices is found to be zero. This arises due to the symmetry of the two copper sub-lattices with impurity f-level lying on the Fermi level. On similar grounds the mixed superconducting pairing amplitudes like $\left\langle a^{\dagger}_{k,\uparrow} f^{\dagger}_{1,-k,\downarrow}\right\rangle$ formed due to the operator of copper at one site and that of the corresponding f impurity level also vanishes. The non-vanishing amplitudes are calculated below and their impact on the SC and AFM order parameters (Δ and h) are to be investigated in the present communications. The mixed amplitude due to operators of intersites of copper atom is given by

$$S_1 = \sum_{k,\sigma}\left[\left\langle a^{\dagger}_{k\uparrow,\sigma} b_{k\uparrow,\sigma}\right\rangle + \left\langle b^{\dagger}_{k\uparrow,\sigma} a_{k\uparrow,\sigma}\right\rangle\right],$$

$$S_1 = \sum_{k,\sigma} \frac{1}{2(\omega_3^2-\omega_2^2)}\{F_{31}-F_{32}\} + \frac{1}{2(\omega_3^2-\omega_4^2)}\{F_{33}-F_{34}\}\Big|, \tag{13}$$

where

$$F_{3i}(i=1-4) = \omega_i \in_k \tanh\left(\frac{1}{2}\beta\omega_i\right).$$

The mixed amplitude due to operators of copper sublattices and that of the corresponding impurity f-level (*i.e.* hybridization strength) is given by

$$S_2 = \sum_{k,\sigma}\left[\left\langle a^{\dagger}_{k\uparrow,\sigma} f_{1,k\uparrow,\sigma}\right\rangle + \left\langle b^{\dagger}_{k\uparrow,\sigma} f_{2,k\uparrow,\sigma}\right\rangle\right],$$

$$S_2 = \sum \frac{1}{4\left(\omega_1^2-\omega_2^2\right)}\{F_{41}-F_{42}\} + \frac{1}{4\left(\omega_3^2-\omega_4^2\right)}\{F_{43}-F_{44}\} \tag{14}$$

where

$$F_{4i}(i=1-4) = \frac{V\left(\omega_i^2-V^2\right)}{\omega_i}\tanh\left(\frac{1}{2}\beta\omega_i\right).$$

The superconducting pairing amplitude due to f-electron sublattice is given by

$$Z_1 = \sum_k\left[\left\langle f^{\dagger}_{1,k\uparrow} f^{\dagger}_{1,-k\downarrow}\right\rangle + \left\langle f^{\dagger}_{2,k\uparrow} f^{\dagger}_{2,-k\downarrow}\right\rangle\right],$$

$$Z_1 = \sum \frac{V^2(h/2-\Delta)}{2\left(\omega_1^2-\omega_2^2\right)}\{F_{51}-F_{52}\} - \frac{V^2(h/2+\Delta)}{2\left(\omega_3^2-\omega_4^2\right)}\{F_{53}-F_{54}\} \tag{15}$$

where

$$F_{5i}(i=1-4) = \frac{1}{\omega_i}\tanh\left(\frac{1}{2}\beta\omega_i\right).$$

Different quantities involved are made dimensionless by dividing them by $2t_0$, where $W = 8t_0$ is the width of the conduction band. They are

$$\frac{\Delta(T)}{2t_0} = Z,\ \frac{\omega_D}{2t_0} = \tilde{\omega}_D,\ \frac{k_B T}{2t_0} = t,\ \frac{h}{2t_0} = h,$$

$$\frac{V}{2t_0} = \upsilon,\ g = N(0)V_0,\ g_1 = N(0)\frac{g\mu_B}{2}.$$

5. Results and discussion

The effect of hybridization (υ) between copper d-electrons and impurity levels ϵ_f on AFM order parameter and SC order parameter z on their co-existence phase is shown in Figure 1. With increase of hybridization, the SC transition temperature t_c is suppressed a little but the Neél temperature (t_N) is reduced considerable amount with increase of the strength of hybridization. However. in the co-existence region, the hybridization has little effect on SC order parameter which almost remains unaffected. The AFM parameter is drastically reduced with increase of the strength of impurity concentration (*i.e.* with increase of hybridization) as shown by experimental observation of phase diagram.

In order to explain the low temperature anomaly in SC order parameter, the temperature dependence hybridization strength S_2 and SC pairing amplitude Z_1 of f-electrons are shown in Figures 2 and 3. It is seen that Z_1 and S_2 have some influence on the SC parameter Z. The mixed amplitude parameter S_1 given in eq. (13) appears due to the hybridization between electron orbitals of the intersite copper atoms. Its temperature variation is negligible small at low temperatures (not shown in figure.)

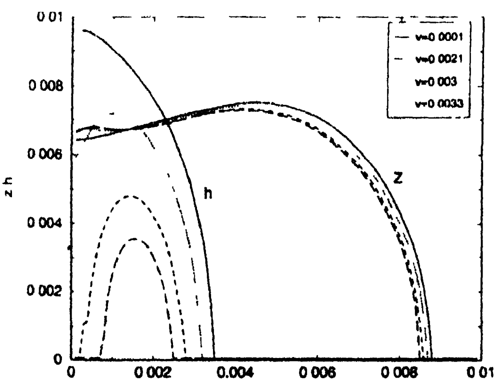

Figure 1. The self-consistent plot of Z, h *vs.* t for fixed values of g = 0.16, g_1 = 0.18 taking different values of V.

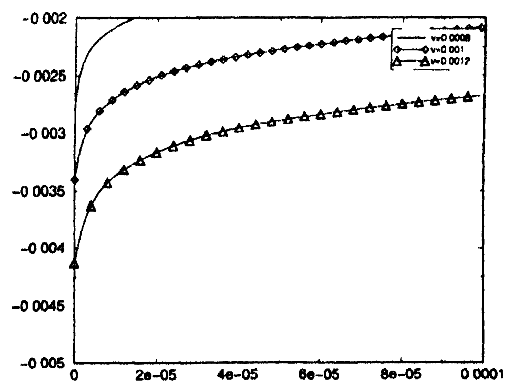

Figure 2. The variation of S_2 *vs.* t for fixed values of g = 0.16 and g_1 = 0.18 taking different values of V.

The mixed amplitude S_2 is due to the hybridization between the electron orbitals of copper sublattices and that of the corresponding impurity f-level. The temperature dependence of S_2 is shown in Figure 2. This mixed amplitude bears a negative value. As temperature increases the value of S_2 increases towards higher temperature. With

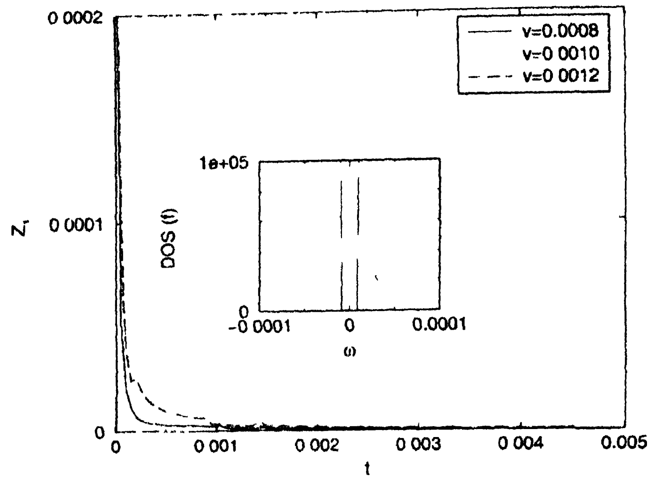

Figure 3. The variation of Z_1 *vs* t for fixed values of g = 0 16 and g_1 = 0 18 taking different values of V

increases of hybridization V = 0.0008 to 0.0012, the parameter S_2 shows more negative value through out the temperature. This hybridization between *d* electrons and *f* electrons induces pair breaking in the superconducting gap, arising due to conduction electrons of copper atoms. As a result, the superconducting parameter Z decreases through out the temperature range due to the pair breaking. Moreover, the stronger negative value of S_2 at low temperatures drastically destroys anti-ferromagnetic order at low temperature as well as through out the temperature range of Neél order. So we observe re-entrant behavior in antiferromagnetism, leading two Neél temperatures *i.e.* t_{N_1} at low temperatures and t_{N_2} at higher temperatures. So anti-ferromagnetism exists within the narrow temperature range $(t_{N_1} < t < t_{N_2})$. The mixed SC pairing amplitude arising due to two *f*-electron sub-lattices is Z_1. The effect of hybridization on the temperature dependence of *f*-electron pairing amplitude Z_1 is shown in Figure 3. The *f*-electron pairing amplitude Z_1 decreases with temperature within the co-existence phase upto Neél temperature t_N. Hence the induced SC in *f*-electron is responsible for the decrease in SC order parameter Z at the low temperatures in co-existence phase. This parameter induces pair breaking SC parameter Z as well as breaking of anti-ferromagnetism order at low temperatures.The *f*-electron density of state, DOS(*f*) is denned as $DOS(f) = \sum_{k,\sigma} \rho^{\alpha}_{k,\sigma}$ where the *f*-electron spectral density function is $\rho^{\alpha}_{k,\sigma} = -2\pi I_m F(k,\omega)$ as the *f*-electron Green's function. The *f*-electron density of state for different conduction band energy is shown in the inset of the Figure 3. Since the impurity *f* electron lies at the Fermi level, we observe a highly peaked (magnitude of the order of 100000 units) *f*-electron density of state near Fermi level ϵ_F = 0. This peak density splits into two, separated by a induced *f* electron narrow superconducting gap of weak amplitude Z_1.

The conclusion is described below.

The self-consistent numerical calculation presents the interplay between antiferromagnetism and superconductivity. The hybridization strength induces pair breaking in the SC order parameter and also drastically destroying magnetization as seen by experimental observation. The mixing hybridization strength S_2 and the induced pairing amplitude Z_1 explain the apparent reduction of the SC and antiferromagnetic orders.

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